2-Chloroethanol 107-07-3 | DTXSID1021877

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 8.66

Global applicability domain: Inside

Local applicability domain index: 4.41e-01

Confidence level: 6.62e-01

Nearest Neighbors from the Training Set

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2-Chloropyridine Measured: 19.1 Predicted: 6.11 Image not found

Allyl chloride Measured: 5.01 Predicted: 6.46 Image not found

Bis(2-chloroethyl) ether Measured: 10.0 Predicted: 9.54

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3-Chloroaniline Measured: 2.24 Predicted: 7.18 Image not found

3-Chlorobenzyl alcohol

Measured: 19.5 Predicted: 7.92